2-Chloronaphthalene 91-58-7 | DTXSID8023971

Model Performance

Model	Data	
IVIOGEI	Dala	

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 52.1

Global applicability domain: Inside

Local applicability domain index: 5.04e-01

Confidence level: 6.06e-01

Nearest Neighbors from the Training Set

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Predicted: 10.1

3,4-Dichloro-1-butene **Measured:** 12.9

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1,2-Dibromo-3-chloropropane

Measured: 11.5 Predicted: 12.9

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1,2,2,3-Tetrachloropropane

Measured: 37.2 Predicted: 20.8

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bis(2-Chloro-1-methylethyl) ether

Measured: 12.0 Predicted: 9.79

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Dieldrin

Measured: 8130 Predicted: 4890

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Endrin

Measured: 8130 Predicted: 4890